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(M25-PS4-20185) Desing, synthesis and antitrichinellosis activity of 1,3-disubsituted benzimidazol-2-ones

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Benzimidazole anthelmintic drugs as thiabendazole, mebendazole, albendazole, etc. are widely used in veterinary and human medicine. Because of their high efficacy, prolonged use of these compounds has led to the development of resistance by many helminth strains.
For this reason, the need for the design and synthesis of new benzimidazole molecules to overcome existing resistance has increased.
Novel 1,3-disubsituted benzimidazol-2-ones were prepared using a multi-step synthetic approach that started from 4-substituded-1,2-diaminobenzenes. The structures of the targeted compounds were confirmed by IR and ^{1}H NMR spectra. In addition, the molecular geometry and electron structure of these molecules were theoretically evaluated using density functional theory (DFT) methods.
The compounds exhibited remarkable activity *in vitro* against isolated Trichinella spiralis muscle larvae.

Keywords: 1,3-disubsituted benzimidazol-2-ones, antitrichinellosis activity; DFT

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(M26-PS4-20190) DFT and experimental IR study on the conversion of 6(7)-nitro-[1,3]thiazolo[3,2-a]-benzimidazole-3(2H)-ones with antiparasitic activity into anion products

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Nitroheterocyclic drugs ability to generate free radicals under anaerobic growth conditions, thus affecting multiple cellular pathways, has been is a successful strategy to develop effective drugs for treatment of parasitic worm infestations. Nitroheterocyclic medications are widely used to cure giardiasis, trichuriasis, filariasis, neurocysticercosis, hydatid disease, pinworm disease, ascariasis, Chagas disease and African sleeping sickness [1,2].

As part of our research on antiparasitic benzimidazole derivatives, various groups of benzimidazole derivatives were synthesized and evaluated for their activity *in vitro* and *in vivo* against different protozoa. The 2-arilyden-thiazolo[3,2-*a*]benzimidazol-3(2*H*)-ones containing different substituents at the 6(7)-position showed remarkable activity against the intestinal and muscle phases of *Trichinella spiralis* in white mice [3]. Having in mind the key role of the nitro group for manifestation of antiparasitic activity, recently we focused our attention on characterizing the metabolites resulting from bioreduction of nitrobenzimidazoles into more details. The possible conversion of nitro compounds into radical anion species can be conveniently studied by electrochemical reduction coupled with IR spectroscopy measurements and quantum chemical calculations on the structure, vibrational spectra and ability of the molecules to accept electrons [4]. Herein we report the results on the electrochemical reduction of some representative 6(7)-nitro-[1,3]thiazolo[3,2-a]-benzimidazole-3(2H)-one derivatives. Molecular structure, electronic charge distribution, vibrational spectra and molecular parameters related to nitro reduction were studied by DFT calculations.

Keywords: Nitrobenzimidazoles, antiparasitic activity, IR study, DFT

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